10/505,257C Yong Chu 1/26/2007

$%^STN;HighlightOn=;HighlightOff=;

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LOGINID:ssptaylc1626

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	OCT 23	The Derwent World Patents Index suite of databases on STN has been enhanced and reloaded
NEWS	4	OCT 30	CHEMLIST enhanced with new search and display field
NEWS	5	NOV 03	JAPIO enhanced with IPC 8 features and functionality
NEWS	6	NOV 10	CA/CAplus F-Term thesaurus enhanced
NEWS	7	NOV 10	STN Express with Discover! free maintenance release Version 8.01c now available
NEWS	8	NOV 20	CAS Registry Number crossover limit increased to 300,000 in additional databases
NEWS	9	NOV 20	CA/CAplus to MARPAT accession number crossover limit increased to 50,000
NEWS	10	DEC 01	CAS REGISTRY updated with new ambiguity codes
NEWS	11	DEC 11	CAS REGISTRY chemical nomenclature enhanced
NEWS	12	DEC 14	WPIDS/WPINDEX/WPIX manual codes updated
NEWS	13	DEC 14	GBFULL and FRFULL enhanced with IPC 8 features and functionality
NEWS	14	DEC 18	CA/CAplus pre-1967 chemical substance index entries enhanced with preparation role
NEWS	15	DEC 18	CA/CAplus patent kind codes updated
NEWS	16	DEC 18	MARPAT to CA/CAplus accession number crossover limit increased to 50,000
NEWS	17	DEC 18	MEDLINE updated in preparation for 2007 reload
NEWS	18	DEC 27	CA/CAplus enhanced with more pre-1907 records
NEWS	19	JAN 08	CHEMLIST enhanced with New Zealand Inventory of Chemicals
NEWS	20	JAN 16	CA/CAplus Company Name Thesaurus enhanced and reloaded
NEWS	21	JAN 16	IPC version 2007.01 thesaurus available on STN
NEWS	22	JAN 16	WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data
NEWS	23	JAN 22	CA/CAplus updated with revised CAS roles
NEWS	24	JAN 22	CA/CAplus enhanced with patent applications from India

NEWS EXPRESS	NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

NEWS X25 X.25 communication option no longer available

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 08:49:12 ON 26 JAN 2007

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.63	0.63

FILE 'REGISTRY' ENTERED AT 08:50:53 ON 26 JAN 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 24 JAN 2007 HIGHEST RN 918400-64-3
DICTIONARY FILE UPDATES: 24 JAN 2007 HIGHEST RN 918400-64-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

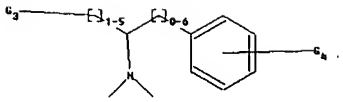
TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

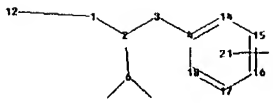
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Documents and Settings\ychu\Desktop\Case\10505257\10505257C.str





chain nodes :
1 2 3 5 6 7 12 20
ring nodes :
4 14 15 16 17 18
chain bonds :
1-2 1-12 2-3 2-6 3-4 5-6 6-7
ring bonds :
4-14 4-18 14-15 15-16 16-17 17-18
exact/norm bonds :
1-12 2-6 5-6 6-7
exact bonds :
1-2 2-3 3-4
normalized bonds :
4-14 4-18 14-15 15-16 16-17 17-18

G1:H,Ak

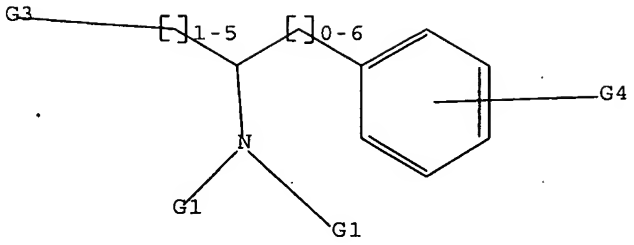
G3:CO2H,PO3H2,SO3H,P,Hy

G4:C,O,S,N

Match level :
1:CLASS 2:CLASS 3:CLASS 4:Atom 5:CLASS 6:CLASS 7:CLASS 12:CLASS 14:Atom
15:Atom 16:Atom 17:Atom 18:Atom 20:CLASS 21:Atom

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



G1 H,Ak
G2
G3 CO2H,PO3H2,SO3H,P,Hy
G4 C,O,S,N

Structure attributes must be viewed using STN Express query preparation.

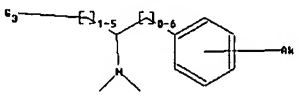
```
=> s l1
SAMPLE SEARCH INITIATED 08:51:22 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   403503 TO ITERATE

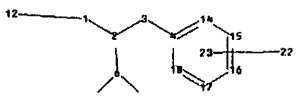
  0.5% PROCESSED     2000 ITERATIONS                                 5 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **INCOMPLETE**
PROJECTED ITERATIONS:      8033707 TO  8106413
PROJECTED ANSWERS:           18270 TO    22080

L2             5 SEA SSS SAM L1

=>
Uploading C:\Documents and Settings\ychu\Desktop\Case\10505257\10505257C-1.str .
```





```
chain nodes :
1  2  3  5  6  7  12  22
ring nodes :
4  14  15  16  17  18
chain bonds :
1-2  1-12  2-3  2-6  3-4  5-6  6-7
ring bonds :
```

4-14 4-18 14-15 15-16 16-17 17-18
exact/norm bonds :
1-12 2-6 5-6 6-7
exact bonds :
1-2 2-3 3-4
normalized bonds :
4-14 4-18 14-15 15-16 16-17 17-18

G1:H,Ak

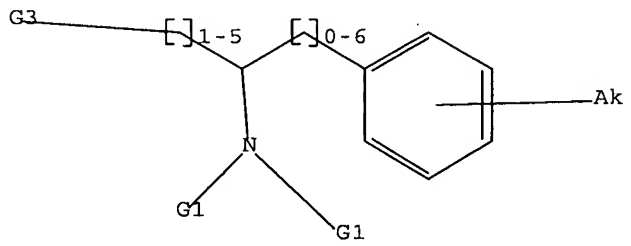
G3:CO2H,PO3H2,SO3H,P,Hy

G4:C,O,S,N

Match level :
1:CLASS 2:CLASS 3:CLASS 4:Atom 5:CLASS 6:CLASS 7:CLASS 12:CLASS 14:Atom
15:Atom 16:Atom 17:Atom 18:Atom 22:CLASS 23:CLASS

L3 STRUCTURE UPLOADED

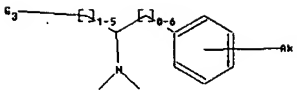
=> d
L3 HAS NO ANSWERS
L3 STR

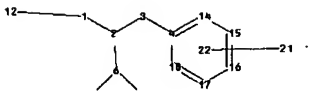


G1 H,Ak
G2
G3 CO2H,PO3H2,SO3H,P,Hy
G4 C,O,S,N

Structure attributes must be viewed using STN Express query preparation.

=>
Uploading C:\Documents and Settings\ychu\Desktop\Case\10505257\10505257C-2.str





chain nodes :
1 2 3 5 6 7 12 21
ring nodes :
4 14 15 16 17 18
chain bonds :
1-2 1-12 2-3 2-6 3-4 5-6 6-7
ring bonds :
4-14 4-18 14-15 15-16 16-17 17-18
exact/norm bonds :
1-12 2-6 5-6 6-7
exact bonds :
1-2 2-3 3-4
normalized bonds :
4-14 4-18 14-15 15-16 16-17 17-18

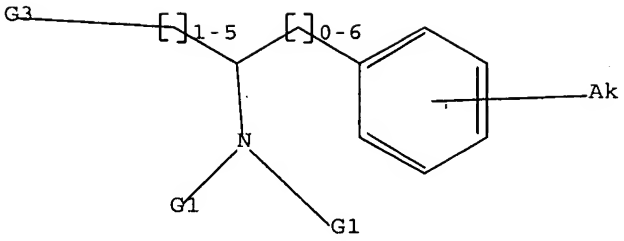
G1:H,Ak

G3:CO2H,PO3H2,SO3H,P,Hy

Match level :
1:CLASS 2:CLASS 3:CLASS 4:Atom 5:CLASS 6:CLASS 7:CLASS 12:CLASS 14:Atom
15:Atom 16:Atom 17:Atom 18:Atom 21:CLASS 22:CLASS

L4 STRUCTURE UPLOADED

=> d
L4 HAS NO ANSWERS
L4 STR



G1 H,Ak
G2
G3 CO2H,PO3H2,SO3H,P,Hy

Structure attributes must be viewed using STN Express query preparation.

=> s l4
SAMPLE SEARCH INITIATED 08:56:24 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 403493 TO ITERATE

0.5% PROCESSED 2000 ITERATIONS 1 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: 8033507 TO 8106213
PROJECTED ANSWERS: 3182 TO 4886

L5 1 SEA SSS SAM L4

=>
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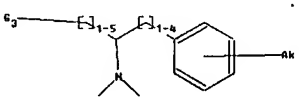
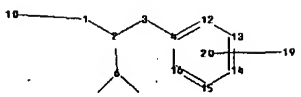




chain nodes :
1 2 3 5 6 7 10 19
ring nodes :
4 12 13 14 15 16
chain bonds :
1-2 1-10 2-3 2-6 3-4 5-6 6-7
ring bonds :
4-12 4-16 12-13 13-14 14-15 15-16

exact/norm bonds :
1-10 2-6 5-6 6-7
exact bonds :
1-2 2-3 3-4
normalized bonds :
4-12 4-16 12-13 13-14 14-15 15-16

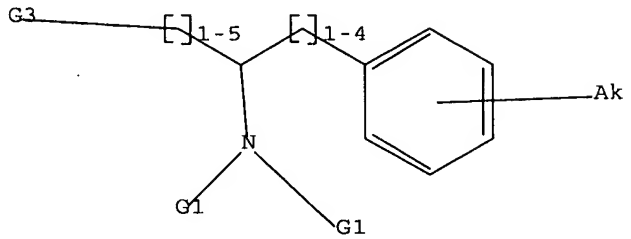
G1:H,Ak

G3:CO2H,PO3H2,SO3H,P,Hy

Match level :
1:CLASS 2:CLASS 3:CLASS 4:Atom 5:CLASS 6:CLASS 7:CLASS 10:CLASS 12:Atom
13:Atom 14:Atom 15:Atom 16:Atom 19:CLASS 20:CLASS

L6 STRUCTURE UPLOADED

=> d
L6 HAS NO ANSWERS
L6 STR



G1 H,Ak
G2
G3 CO2H,PO3H2,SO3H,P,Hy

Structure attributes must be viewed using STN Express query preparation.

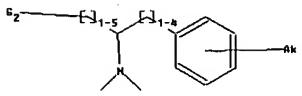
=> s l6
SAMPLE SEARCH INITIATED 08:57:41 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 149459 TO ITERATE

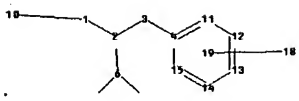
1.3% PROCESSED 2000 ITERATIONS 5 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: 2966375 TO 3011985
PROJECTED ANSWERS: 6313 TO 8631

L7 5 SEA SSS SAM L6

=>
Uploading C:\Documents and Settings\ychu\Desktop\Case\10505257\10505257C-4.str





chain nodes :
1 2 3 5 6 7 10 18
ring nodes :
4 11 12 13 14 15
chain bonds :
1-2 1-10 2-3 2-6 3-4 5-6 6-7
ring bonds :
4-11 4-15 11-12 12-13 13-14 14-15
exact/norm bonds :
1-10 2-6 5-6 6-7
exact bonds :
1-2 2-3 3-4
normalized bonds :
4-11 4-15 11-12 12-13 13-14 14-15

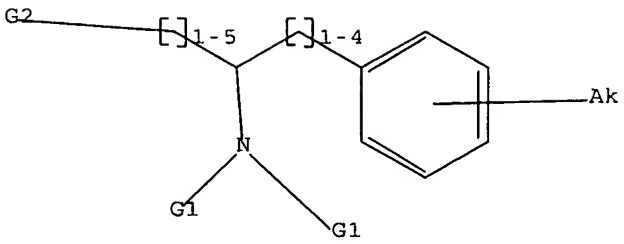
G1:H,Ak

G2:CO2H,PO3H2,SO3H,P

Match level :
1:CLASS 2:CLASS 3:CLASS 4:Atom 5:CLASS 6:CLASS 7:CLASS 10:CLASS 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 18:CLASS 19:CLASS

L8 STRUCTURE UPLOADED

=> d
L8 HAS NO ANSWERS
L8 STR



G1 H,Ak
G2 CO2H,PO3H2,SO3H,P

Structure attributes must be viewed using STN Express query preparation.

```
=> s l8
SAMPLE SEARCH INITIATED 09:03:18 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    40869 TO ITERATE

  4.9% PROCESSED     2000 ITERATIONS                              0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       805306 TO   829454
PROJECTED ANSWERS:               0 TO        0

L9             0 SEA SSS SAM L8

=> s l8 full
FULL SEARCH INITIATED 09:05:01 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   818627 TO ITERATE

 75.4% PROCESSED   616890 ITERATIONS                            252 ANSWERS

 97.7% PROCESSED   799886 ITERATIONS                            306 ANSWERS

 98.9% PROCESSED   809895 ITERATIONS                            318 ANSWERS

100.0% PROCESSED   818627 ITERATIONS                            318 ANSWERS
SEARCH TIME: 00.00.53

L10          318 SEA SSS FUL L8

=> file caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                              183.35     183.98

FILE 'CAPLUS' ENTERED AT 09:06:12 ON 26 JAN 2007
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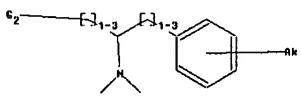
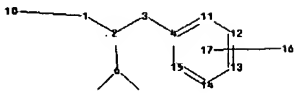
FILE COVERS 1907 - 26 Jan 2007 VOL 146 ISS 6
FILE LAST UPDATED: 25 Jan 2007 (20070125/ED)

=> s l10
L11 94 L10

=>
Uploading C:\Documents and Settings\ychu\Desktop\Case\10505257\10505257C-5.str





chain nodes :
1 2 3 5 6 7 10 16
ring nodes :
4 11 12 13 14 15
chain bonds :
1-2 1-10 2-3 2-6 3-4 5-6 6-7
ring bonds :
4-11 4-15 11-12 12-13 13-14 14-15
exact/norm bonds :
1-10 2-6 5-6 6-7
exact bonds :
1-2 2-3 3-4
normalized bonds :
4-11 4-15 11-12 12-13 13-14 14-15

G1:H,Ak

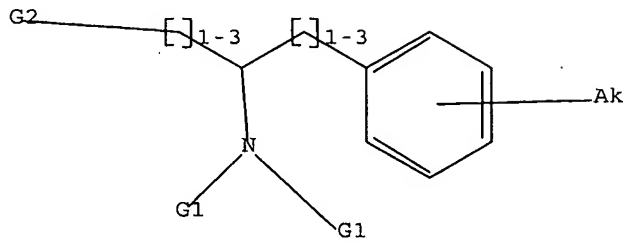
G2:CO2H,PO3H2,SO3H,P

Match level :
1:CLASS 2:CLASS 3:CLASS 4:Atom 5:CLASS 6:CLASS 7:CLASS 10:CLASS 11:Atom

12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS

L12   STRUCTURE UPLOADED

=> d
L12 HAS NO ANSWERS
L12   STR



G1 H,Ak
G2 CO2H,PO3H2,SO3H,P

Structure attributes must be viewed using STN Express query preparation.

=> s l12
   REGISTRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 09:12:35 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   40869 TO ITERATE

  4.9% PROCESSED   2000 ITERATIONS   0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS: 805306 TO   829454
PROJECTED ANSWERS: 0 TO   0

L13   0 SEA SSS SAM L12

L14   0 L13

=> file reg
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                 ENTRY   SESSION

FULL ESTIMATED COST 0.47 190.07

FILE 'REGISTRY' ENTERED AT 09:12:46 ON 26 JAN 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 24 JAN 2007 HIGHEST RN 918400-64-3
DICTIONARY FILE UPDATES: 24 JAN 2007 HIGHEST RN 918400-64-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

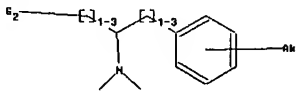
TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

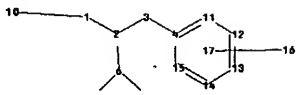
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Documents and Settings\ychu\Desktop\Case\10505257\10505257C-5.str





chain nodes :
1 2 3 5 6 7 10 16
ring nodes :
4 11 12 13 14 15
chain bonds :
1-2 1-10 2-3 2-6 3-4 5-6 6-7
ring bonds :
4-11 4-15 11-12 12-13 13-14 14-15
exact/norm bonds :
1-10 2-6 5-6 6-7
exact bonds :
1-2 2-3 3-4
normalized bonds :
4-11 4-15 11-12 12-13 13-14 14-15

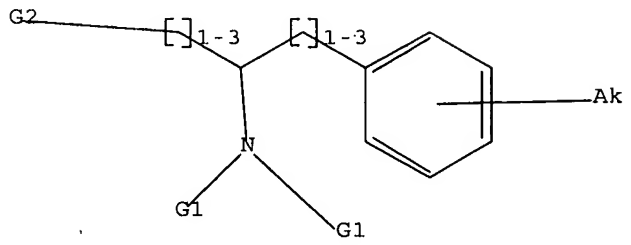
G1:H,Ak

G2:CO2H,PO3H2,SO3H,P

Match level :
1:CLASS 2:CLASS 3:CLASS 4:Atom 5:CLASS 6:CLASS 7:CLASS 10:CLASS 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS

L15 STRUCTURE UPLOADED

=> d
L15 HAS NO ANSWERS
L15 STR



G1 H,Ak
G2 CO2H,PO3H2,SO3H,P

Structure attributes must be viewed using STN Express query preparation.

=> s l15
SAMPLE SEARCH INITIATED 09:13:08 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 40869 TO ITERATE

4.9% PROCESSED 2000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 805306 TO 829454
PROJECTED ANSWERS: 0 TO 0

L16 0 SEA SSS SAM L15

=> s l15
SAMPLE SEARCH INITIATED 09:13:28 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 40869 TO ITERATE

4.9% PROCESSED 2000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

```
                        BATCH    **COMPLETE**
PROJECTED ITERATIONS:        805306 TO   829454
PROJECTED ANSWERS:                0 TO        0

L17           0 SEA SSS SAM L15

=> s l15 full
FULL SEARCH INITIATED 09:13:42 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    818627 TO ITERATE

 87.3% PROCESSED    714743 ITERATIONS                                288 ANSWERS

 98.8% PROCESSED    808958 ITERATIONS                                313 ANSWERS

100.0% PROCESSED    818627 ITERATIONS                                313 ANSWERS
SEARCH TIME: 00.00.39

L18         313 SEA SSS FUL L15

=> file caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                     173.00     363.07

FILE 'CAPLUS' ENTERED AT 09:14:43 ON 26 JAN 2007
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FILE COVERS 1907 - 26 Jan 2007  VOL 146 ISS 6
FILE LAST UPDATED: 25 Jan 2007  (20070125/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l18
L19          94 L18

=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       1.41     364.48

FILE 'REGISTRY' ENTERED AT 09:16:26 ON 26 JAN 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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```

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 24 JAN 2007 HIGHEST RN 918400-64-3
DICTIONARY FILE UPDATES: 24 JAN 2007 HIGHEST RN 918400-64-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

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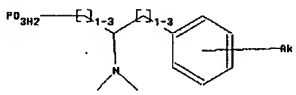
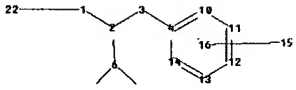
Uploading C:\Documents and Settings\ychu\Desktop\Case\10505257\10505257C-6.str





chain nodes :
1 2 3 5 6 7 15 22
ring nodes :
4 10 11 12 13 14
chain bonds :
1-2 1-22 2-3 2-6 3-4 5-6 6-7
ring bonds :
4-10 4-14 10-11 11-12 12-13 13-14
exact/norm bonds :
2-6 5-6 6-7
exact bonds :
1-2 1-22 2-3 3-4
normalized bonds :
4-10 4-14 10-11 11-12 12-13 13-14

G1:H,Ak

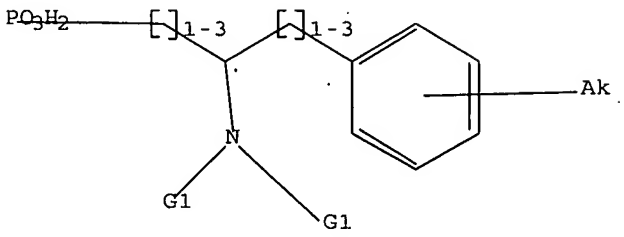
G2:CO2H,PO3H2,SO3H,P

Match level :
1:CLASS 2:CLASS 3:CLASS 4:Atom 5:CLASS 6:CLASS 7:CLASS 10:Atom 11:Atom

12:Atom
13:Atom 14:Atom 15:CLASS 16:CLASS 22:CLASS

L20 STRUCTURE UPLOADED

=> d
L20 HAS NO ANSWERS
L20 STR



G1 H,Ak
G2 CO2H,PO3H2,SO3H,P

Structure attributes must be viewed using STN Express query preparation.

=> s l20
SAMPLE SEARCH INITIATED 09:16:56 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 72 TO ITERATE

100.0% PROCESSED 72 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                        BATCH **COMPLETE**
PROJECTED ITERATIONS: 931 TO 1949
PROJECTED ANSWERS: 2 TO 124

L21 2 SEA SSS SAM L20

=> s l20 full
FULL SEARCH INITIATED 09:17:09 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1470 TO ITERATE

100.0% PROCESSED 1470 ITERATIONS 37 ANSWERS
SEARCH TIME: 00.00.01

L22 37 SEA SSS FUL L20

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 172.10 536.58

FILE 'CAPLUS' ENTERED AT 09:17:16 ON 26 JAN 2007

FILE COVERS 1907 - 26 Jan 2007 VOL 146 ISS 6
FILE LAST UPDATED: 25 Jan 2007 (20070125/ED)

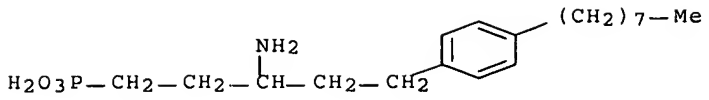
=> s l22
L23 8 L22

=> d ibib abs hitstr tot

L23 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:465499 CAPLUS Full-text
DOCUMENT NUMBER: 141:133550
TITLE: The discovery of 3-(N-alkyl)aminopropylphosphonic acids as potent S1P receptor agonists
AUTHOR(S): Hale, Jeffrey J.; Doherty, George; Toth, Leslie; Li, Zhen; Mills, Sander G.; Hajdu, Richard; Keohane, Carol Ann; Rosenbach, Mark; Milligan, James; Shei, Gan-Ju; Chrebet, Gary; Bergstrom, James; Card, Deborah; Rosen, Hugh; Mandala, Suzanne
CORPORATE SOURCE: Department of Medicinal Chemistry, Merck Research Laboratories, Rahway, NJ, 07065, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(13), 3495-3499
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:133550

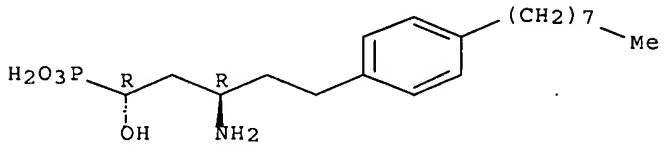
AB 3-(N-Alkyl)aminopropylphosphonic acids are potent agonists of four of the five known sphingosine-1-phosphate (S1P) receptor subtypes and are useful in immunosuppressive therapy.

IT 596819-84-0 597340-18-6
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(prepn., immunomodulatory effect and structure-activity relationship studies of 3-(N-alkyl)aminopropylphosphonic acids as potent S1P receptor agonists)
RN 596819-84-0 CAPLUS
CN Phosphonic acid, [3-amino-5-(4-octylphenyl)pentyl]- (9CI) (CA INDEX NAME)



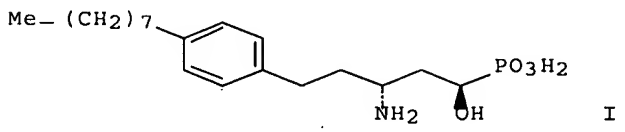
RN 597340-18-6 CAPLUS
CN Phosphonic acid, [(1R,3R)-3-amino-1-hydroxy-5-(4-octylphenyl)pentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:403930 CAPLUS Full-text
DOCUMENT NUMBER: 141:99305
TITLE: Potent S1P receptor agonists replicate the pharmacologic actions of the novel immune modulator FTY720
AUTHOR(S): Hale, Jeffrey J.; Neway, William; Mills, Sander G.; Hajdu, Richard; Keohane, Carol Ann; Rosenbach, Mark; Milligan, James; Shei, Gan-Ju; Chrebet, Gary; Bergstrom, James; Card, Deborah; Koo, Gloria C.; Koprak, Sam L.; Jackson, Jesse J.; Rosen, Hugh; Mandala, Suzanne
CORPORATE SOURCE: Department of Medicinal Chemistry, Merck Research Laboratories, Rahway, NJ, 07065, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(12), 3351-3355
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

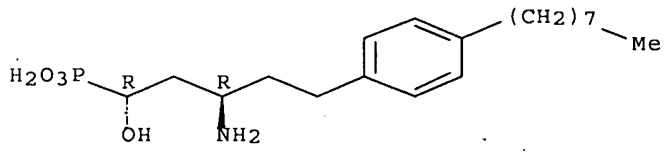
AB Alteration in lymphocyte trafficking and prevention of graft rejection in rodents obsd. on exposure to FTY720 or its corresponding phosphate ester can

be induced by the systemic administration of potent sphingosine-1-phosphate receptor agonists exemplified by I. The similar S1P receptor profiles of the FTY720 phosphate ester and I coupled with their comparable potency in vivo supports a connection between S1P receptor agonism and immunosuppressive efficacy.

IT 597340-18-6P 597340-22-2P 597340-27-7P
597340-33-5P
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(potent sphingosine-1-phosphate receptor agonists replicate the pharmacol. actions of novel immunosuppressant FTY720 in prevention of graft rejection in relation to alteration in lymphocyte trafficking and pharmacokinetics)

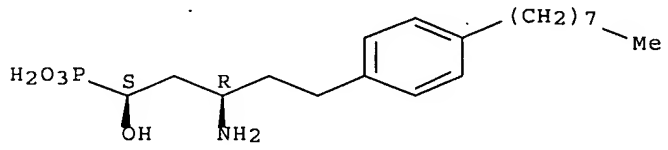
RN 597340-18-6 CAPLUS
CN Phosphonic acid, [(1R,3R)-3-amino-1-hydroxy-5-(4-octylphenyl)pentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



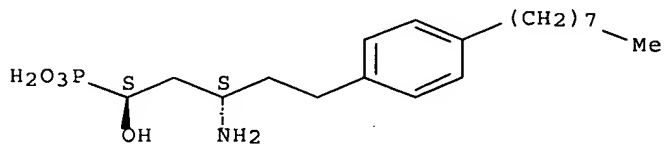
RN 597340-22-2 CAPLUS
CN Phosphonic acid, [(1S,3R)-3-amino-1-hydroxy-5-(4-octylphenyl)pentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



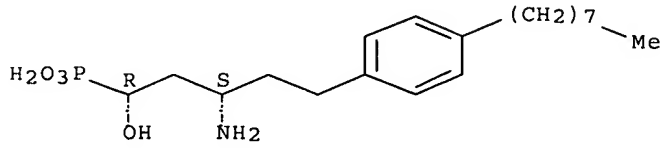
RN 597340-27-7 CAPLUS
CN Phosphonic acid, [(1S,3S)-3-amino-1-hydroxy-5-(4-octylphenyl)pentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



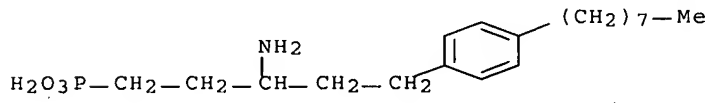
RN 597340-33-5 CAPLUS
CN Phosphonic acid, [(1R,3S)-3-amino-1-hydroxy-5-(4-octylphenyl)pentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

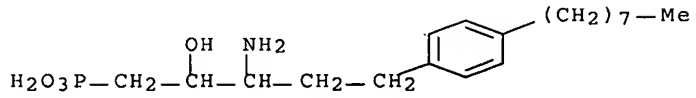


IT 596819-84-0P 596819-85-1P 717888-62-5P 717888-67-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(potent sphingosine-1-phosphate receptor agonists replicate the pharmacol. actions of novel immunosuppressant FTY720 in prevention of graft rejection in relation to alteration in lymphocyte trafficking and pharmacokinetics)

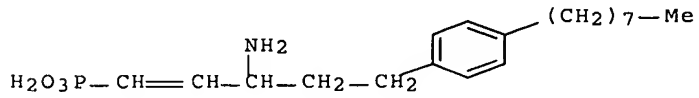
RN 596819-84-0 CAPLUS
CN Phosphonic acid, [3-amino-5-(4-octylphenyl)pentyl]- (9CI) (CA INDEX NAME)



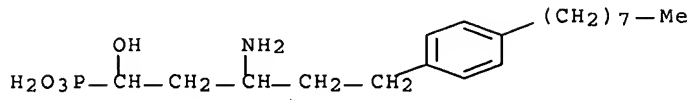
RN 596819-85-1 CAPLUS
CN Pentitol, 3-amino-1,2,3,5-tetradeoxy-1-(4-octylphenyl)-5-phosphono- (9CI) (CA INDEX NAME)



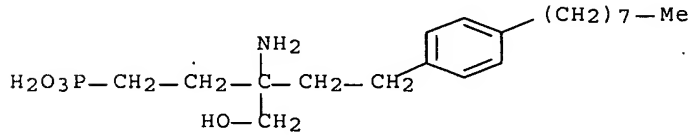
RN 717888-62-5 CAPLUS
CN Phosphonic acid, [3-amino-5-(4-octylphenyl)-1-pentenyl]- (9CI) (CA INDEX NAME)



RN 717888-67-0 CAPLUS
CN Phosphonic acid, [3-amino-1-hydroxy-5-(4-octylphenyl)pentyl]- (9CI) (CA INDEX NAME)



IT 402615-93-4
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(potent sphingosine-1-phosphate receptor agonists replicate the pharmacol. actions of novel immunosuppressant FTY720 in prevention of graft rejection in relation to alteration in lymphocyte trafficking and pharmacokinetics)
RN 402615-93-4 CAPLUS
CN Phosphonic acid, [3-amino-3-(hydroxymethyl)-5-(4-octylphenyl)pentyl]- (9CI) (CA INDEX NAME)



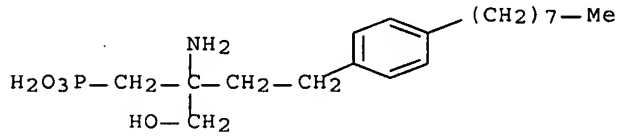
REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:368306 CAPLUS Full-text
DOCUMENT NUMBER: 141:99302
TITLE: Immune cell regulation and cardiovascular effects of sphingosine 1-phosphate receptor agonists in rodents are mediated via distinct receptor subtypes
AUTHOR(S): Forrest, M.; Sun, S.-Y.; Hajdu, R.; Bergstrom, J.; Card, D.; Doherty, G.; Hale, J.; Keohane, C.; Meyers, C.; Milligan, J.; Mills, S.; Nomura, N.; Rosen, H.; Rosenbach, M.; Shei, G.-J.; Singer, I. I.; Tian, M.; West, S.; White, V.; Xie, J.; Proia, R. L.; Mandala, S.
CORPORATE SOURCE: Departments of Immunology and Rheumatology, Pharmacology, and Medicinal Chemistry, Merck Research Laboratories, Rahway, NJ, USA
SOURCE: Journal of Pharmacology and Experimental Therapeutics (2004), 309(2), 758-768
CODEN: JPETAB; ISSN: 0022-3565
PUBLISHER: American Society for Pharmacology and Experimental Therapeutics
DOCUMENT TYPE: Journal
LANGUAGE: English

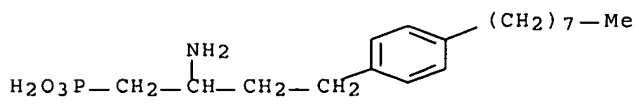
AB Sphingosine 1-phosphate (S1P) is a bioactive lysolipid with pleiotropic functions mediated through a family of G protein-coupled receptors, S1P1,2,3,4,5. Physiol. effects of S1P receptor agonists include regulation of cardiovascular function and immunosuppression via redistribution of lymphocytes from blood to secondary lymphoid organs. The phosphorylated metabolite of the immunosuppressant agent FTY720 (2-amino-2-(2-[4-octylphenyl]ethyl)-1,3-propanediol) and other phosphonate analogs with differential receptor selectivity were investigated. No significant species differences in compd. potency or rank order of activity on receptors cloned from human, murine, and rat sources were obsd. All synthetic analogs were high-affinity agonists on S1P1, with IC50 values for ligand binding between 0.3 and 14 nM. The correlation between S1P1 receptor activation and the ED50 for lymphocyte redn. was highly significant ($p < 0.001$) and lower for the other receptors. In contrast to S1P1-mediated effects on lymphocyte recirculation, three lines of evidence link S1P3 receptor activity with acute toxicity and cardiovascular regulation: compd. potency on S1P3 correlated with toxicity and bradycardia; the shift in potency of phosphorylated-FTY720 for inducing lymphopenia vs. bradycardia and hypertension was consistent with affinity for S1P1 relative to S1P3; and toxicity, bradycardia, and hypertension were absent in S1P3-/- mice. Blood pressure effects of agonists in anesthetized rats were complex, whereas hypertension was the predominant effect in conscious rats and mice. Immunolocalization of S1P3 in rodent heart revealed abundant expression on myocytes and perivascular smooth muscle cells consistent with regulation of bradycardia and hypertension, whereas S1P1 expression was restricted to the vascular endothelium.

IT 719286-66-5 719286-67-6
RL: PAC (Pharmacological activity); BIOL (Biological study)
(immune cell regulation and cardiovascular effects of sphingosine 1-phosphate receptor agonists in rodents are mediated via distinct receptor subtypes)

RN 719286-66-5 CAPLUS
CN Phosphonic acid, [2-amino-2-(hydroxymethyl)-4-(4-octylphenyl)butyl]- (9CI) (CA INDEX NAME)



RN 719286-67-6 CAPLUS
CN Phosphonic acid, [2-amino-4-(4-octylphenyl)butyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:719274 CAPLUS Full-text
DOCUMENT NUMBER: 139:246116
TITLE: Preparation of aminoalkylphosphonates and related compounds as EDG receptor agonists
INVENTOR(S): Doherty, George A.; Hale, Jeffrey J.
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 75 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003074008	A2	20030912	WO 2003-US7262	20030225
WO 2003074008	A3	20040226		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2477449	A1	20030912	CA 2003-2477449	20030225
AU 2003218056	A1	20030916	AU 2003-218056	20030225
EP 1482896	A2	20041208	EP 2003-714037	20030225
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 2005107345	A1	20050519	US 2003-505268	20030225
JP 2005531508	T	20051020	JP 2003-572530	20030225
PRIORITY APPLN. INFO.:			US 2002-360605P P	20020301
			WO 2003-US7262 W	20030225

OTHER SOURCE(S): MARPAT 139:246116

AB The present invention encompasses title compds., A-X[CR1R2]mCHNH2[CR3R4]pC(R9)3 (m = 1-4; p = 9-20; X = bond, O, NH, S(O)k, k = 0-2; A = CO2H, PO3H2, PO2H2, SO3H, five membered nitrogen contg. heterocyclyl, etc.; two R1 or R3 groups on adjacent carbon may be joined together to form a double bond; R2, R3, R4 = H, halo, OH, CO2H, C1-4 alkyl, alkoxy, alkylthio, aryl, etc.; R1-R4 = residing on the same carbon optionally joined together to form a carbonyl group, etc.; R9 = H, halo, OH, C1-4 alkoxy, alkylthio, C3-7 cycloalkyl, etc.); as well as the pharmaceutically acceptable salts and hydrates thereof. The compds. are useful for treating immune mediated diseases and conditions, such as bone marrow, organ and tissue transplant rejection. Pharmaceutical compns. and methods of use are included. Thus, prepn. of (+/-)-2-amino-4-(4- (octylphenyl))butanol, O-phosphate was described in five steps starting from di-Et 2-acetamido-2-(2-(4-octylphenyl)ethyl)propanedioate.

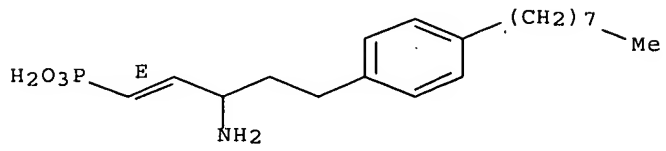
IT 596819-82-8P 596819-84-0P 596819-85-1P
596819-95-3P 596819-96-4P 596819-98-6P
596819-99-7P 596820-00-7P 596820-06-3P
596820-07-4P 596820-16-5P 596820-17-6P
596820-18-7P
RL: ADV (Adverse effect, including toxicity); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of aminoalkylphosphonates and related compds. as EDG receptor

agonists)

RN 596819-82-8 CAPLUS

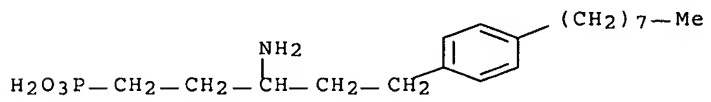
CN Phosphonic acid, [(1E)-3-amino-5-(4-octylphenyl)-1-pentenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



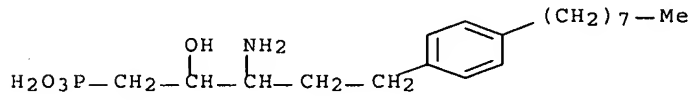
RN 596819-84-0 CAPLUS

CN Phosphonic acid, [3-amino-5-(4-octylphenyl)pentyl]- (9CI) (CA INDEX NAME)



RN 596819-85-1 CAPLUS

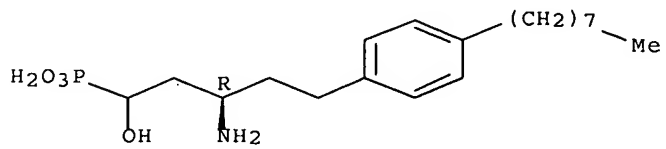
CN Pentitol, 3-amino-1,2,3,5-tetradeoxy-1-(4-octylphenyl)-5-phosphono- (9CI) (CA INDEX NAME)



RN 596819-95-3 CAPLUS

CN Phosphonic acid, [(3R)-3-amino-1-hydroxy-5-(4-octylphenyl)pentyl]- (9CI) (CA INDEX NAME)

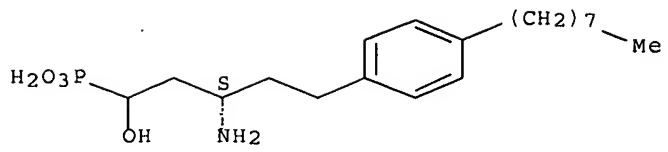
Absolute stereochemistry.



RN 596819-96-4 CAPLUS

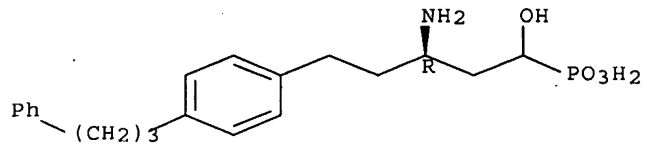
CN Phosphonic acid, [(3S)-3-amino-1-hydroxy-5-(4-octylphenyl)pentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



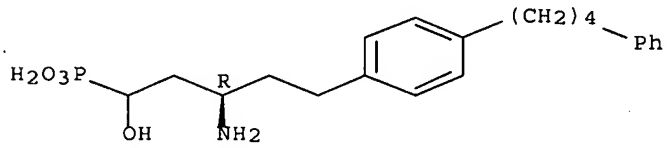
RN 596819-98-6 CAPLUS
CN Phosphonic acid, [(3R)-3-amino-1-hydroxy-5-[4-(3-phenylpropyl)phenyl]pentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



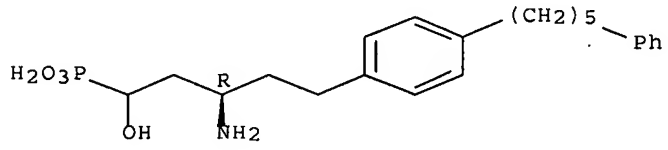
RN 596819-99-7 CAPLUS
CN Phosphonic acid, [(3R)-3-amino-1-hydroxy-5-[4-(4-phenylbutyl)phenyl]pentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



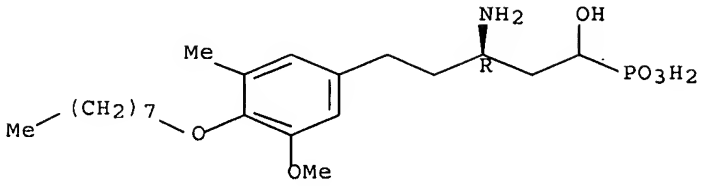
RN 596820-00-7 CAPLUS
CN Phosphonic acid, [(3R)-3-amino-1-hydroxy-5-[4-(5-phenylpentyl)phenyl]pentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



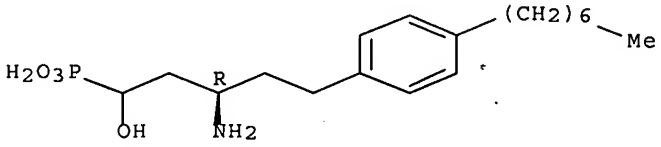
RN 596820-06-3 CAPLUS
CN Phosphonic acid, [(3R)-3-amino-1-hydroxy-5-[3-methoxy-5-methyl-4-(octyloxy)phenyl]pentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

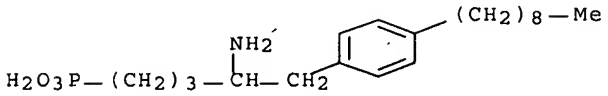


RN 596820-07-4 CAPLUS
CN Phosphonic acid, [(3R)-3-amino-5-(4-heptylphenyl)-1-hydroxypentyl]- (9CI) (CA INDEX NAME)

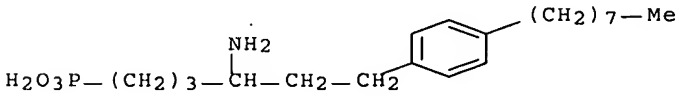
Absolute stereochemistry.



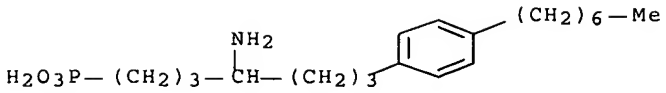
RN 596820-16-5 CAPLUS
CN Phosphonic acid, [4-amino-5-(4-nonylphenyl)pentyl]- (9CI) (CA INDEX NAME)



RN 596820-17-6 CAPLUS
CN Phosphonic acid, [4-amino-6-(4-octylphenyl)hexyl]- (9CI) (CA INDEX NAME)



RN 596820-18-7 CAPLUS
CN Phosphonic acid, [4-amino-7-(4-heptylphenyl)heptyl]- (9CI) (CA INDEX NAME)



L23 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:719253 CAPLUS Full-text
DOCUMENT NUMBER: 139:245479
TITLE: Preparation of aminoalkylphosphonates and related compounds as EDG receptor agonists
INVENTOR(S): Budhu, Richard J.; Doherty, George A.; Hale, Jeffrey J.; Lynch, Christopher L.; Mills, Sander G.; Neway, William E., III
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 90 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

Current app.

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003073986	A2	20030912	WO 2003-US5947	20030227
WO 2003073986	A3	20040527		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2477423	A1	20030912	CA 2003-2477423	20030227
AU 2003217764	A1	20030916	AU 2003-217764	20030227
EP 1482895	A2	20041208	EP 2003-713727	20030227
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2005531506	T	20051020	JP 2003-572508	20030227
US 2006089334	A1	20060427	US 2004-505257	20040819
PRIORITY APPLN. INFO.:			US 2002-360663P P	20020301
			WO 2003-US5947 W	20030227

OTHER SOURCE(S): MARPAT 139:245479

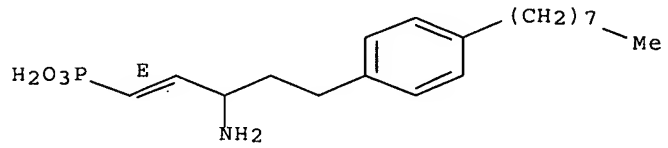
AB AX(CR1R2)mCH(NH2)(CR3R4)nArBC [A = CO2H, P(O)(OH)2, PH(O)(OH),SO3H, P(O)R5OH, 5-membered N heterocycle; X = bond, O, NH, S, S, S(O), SO2; R1-R4 = H, halogen, OH, CO2H, (un)substituted alkyl, alkoxy, alkylthio, aryl; R1R2, R3R4 = O; m = 1-4; n = 0-4; R5 = (un)substituted alkyl, aryl; Ar = Ph, naphthyl; C = (un)substituted alkyl, alkoxy, acyl, hydroxyalkyl, Ph, heterocyclic, bond; when C = bond, B = (un)substituted Ph, alkyl, alkenyl, alkynyl, OH, SH, acyl, CONH2, NH2; when C = Ph, heterocyclic, B = (un)substituted alkyl, alkoxy, acyl, CO, CH(OH), C6H4, heterocyclic; when C = alkyl, alkoxy, acyl, B = (un)substituted C6H4, heterocyclic] were prepd. for use as EDG receptor antagonists useful for treating immune mediated diseases and conditions, such as bone marrow, organ and tissue transplant rejection (no data). Thus, 4-Me(CH2)7C6H4CH2CH2C(NHAc)(CO2Et)2 was hydrolyzed and decarboxylated to 4-

Me(CH2)7C6H4CH2CH2CH(NH2)CO2H which was N-benzyloxycarbonylated, reduced to 4-Me(CH2)7C6H4CH2CH2CH(NHCbz)CH2OH , phosphorylated (MeCH)2NP(OCH2Ph)2, and deblocked to give 4-Me(CH2)7C6H4CH2CH2CH(NH2)CH2OP(O)(OH)2.

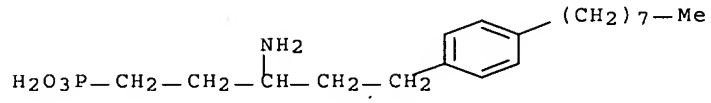
IT 596819-82-8P 596819-84-0P 596819-85-1P
596819-98-6P 596819-99-7P 596820-00-7P
596820-06-3P 596820-07-4P 597340-18-6P
597340-22-2P 597340-27-7P 597340-33-5P
597341-16-7P 597341-24-7P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of aminoalkylphosphonates and related compds. as EDG receptor agonists)

RN 596819-82-8 CAPLUS
CN Phosphonic acid, [(1E)-3-amino-5-(4-octylphenyl)-1-pentenyl]- (9CI) (CA INDEX NAME)

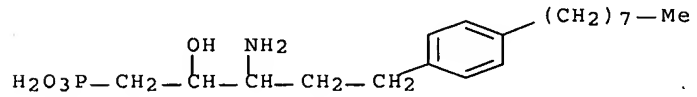
Double bond geometry as shown.



RN 596819-84-0 CAPLUS
CN Phosphonic acid, [3-amino-5-(4-octylphenyl)pentyl]- (9CI) (CA INDEX NAME)

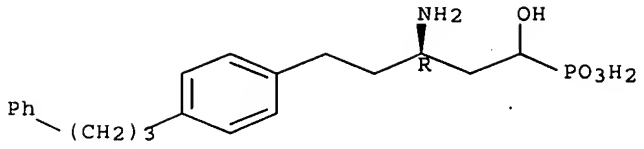


RN 596819-85-1 CAPLUS
CN Pentitol, 3-amino-1,2,3,5-tetradeoxy-1-(4-octylphenyl)-5-phosphono- (9CI) (CA INDEX NAME)



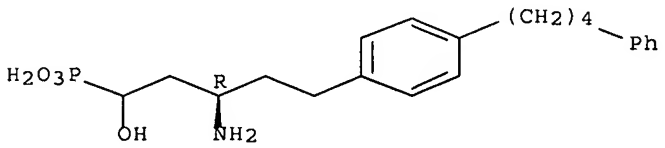
RN 596819-98-6 CAPLUS
CN Phosphonic acid, [(3R)-3-amino-1-hydroxy-5-[4-(3-phenylpropyl)phenyl]pentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



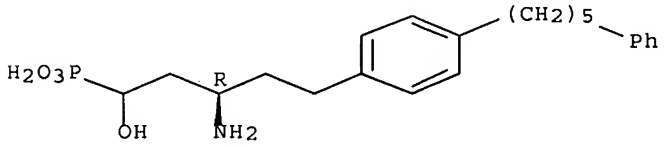
RN 596819-99-7 CAPLUS
CN Phosphonic acid, [(3R)-3-amino-1-hydroxy-5-[4-(4-phenylbutyl)phenyl]pentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



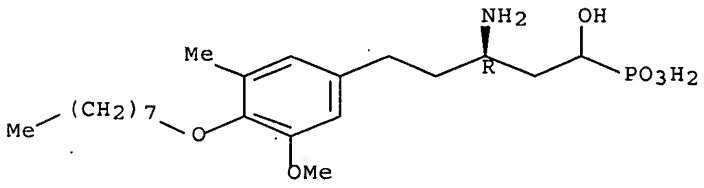
RN 596820-00-7 CAPLUS
CN Phosphonic acid, [(3R)-3-amino-1-hydroxy-5-[4-(5-phenylpentyl)phenyl]pentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



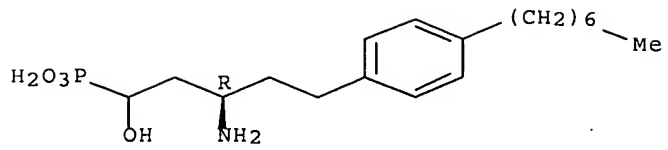
RN 596820-06-3 CAPLUS
CN Phosphonic acid, [(3R)-3-amino-1-hydroxy-5-[3-methoxy-5-methyl-4-(octyloxy)phenyl]pentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



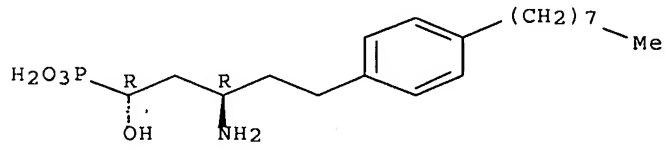
RN 596820-07-4 CAPLUS
CN Phosphonic acid, [(3R)-3-amino-5-(4-heptylphenyl)-1-hydroxypentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



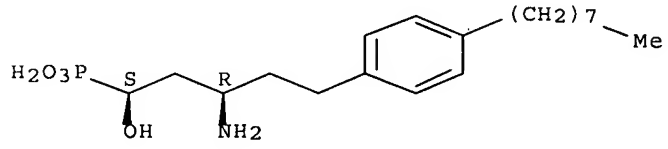
RN 597340-18-6 CAPLUS
CN Phosphonic acid, [(1R,3R)-3-amino-1-hydroxy-5-(4-octylphenyl)pentyl]-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



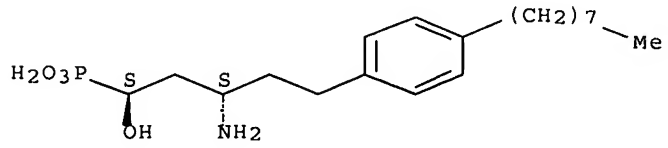
RN 597340-22-2 CAPLUS
CN Phosphonic acid, [(1S,3R)-3-amino-1-hydroxy-5-(4-octylphenyl)pentyl]-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 597340-27-7 CAPLUS
CN Phosphonic acid, [(1S,3S)-3-amino-1-hydroxy-5-(4-octylphenyl)pentyl]-
(9CI) (CA INDEX NAME)

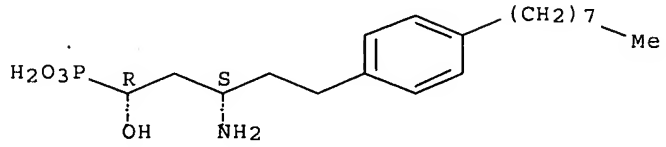
Absolute stereochemistry.



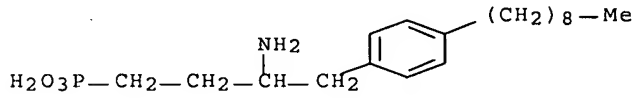
RN 597340-33-5 CAPLUS

CN Phosphonic acid, [(1R,3S)-3-amino-1-hydroxy-5-(4-octylphenyl)pentyl]- (9CI) (CA INDEX NAME)

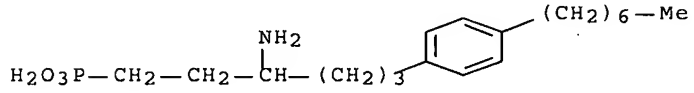
Absolute stereochemistry.



RN 597341-16-7 CAPLUS
CN Phosphonic acid, [3-amino-4-(4-nonylphenyl)butyl]- (9CI) (CA INDEX NAME)



RN 597341-24-7 CAPLUS
CN Phosphonic acid, [3-amino-6-(4-heptylphenyl)hexyl]- (9CI) (CA INDEX NAME)



L23 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:301209 CAPLUS Full-text
DOCUMENT NUMBER: 137:241872
TITLE: Alteration of lymphocyte trafficking by sphingosine-1-phosphate receptor agonists
AUTHOR(S): Mandala, Suzanne; Hajdu, Richard; Bergstrom, James; Quackenbush, Elizabeth; Xie, Jenny; Milligan, James; Thornton, Rosemary; Shei, Gan-Ju; Card, Deborah; Keohane, Carolann; Rosenbach, Mark; Hale, Jeffrey; Lynch, Christopher L.; Rupprecht, Kathleen; Parsons, William; Rosen, Hugh
CORPORATE SOURCE: Departments of Immunology and Rheumatology, Merck Res. Laboratories, Rahway, NJ, 07065, USA
SOURCE: Science (Washington, DC, United States) (2002), 296(5566), 346-349
CODEN: SCIEAS; ISSN: 0036-8075
PUBLISHER: American Association for the Advancement of Science
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Blood lymphocyte nos., essential for the development of efficient immune responses, are maintained by recirculation through secondary Lymphoid organs. We show that lymphocyte trafficking is altered by the lysophospholipid

primary (E)-allylamines, and .beta.-amino phosphine oxides and -phosphonates from .beta.-functionalized oxime derivatives

AUTHOR(S): Palacios, Francisco; Aparicio, Domitila; Garcia, Jesus; Rodriguez, Encina

CORPORATE SOURCE: Departamento Quimica Organica, Facultad Farmacia, Universidad Pais Vasco, Vitoria, E-01080, Spain

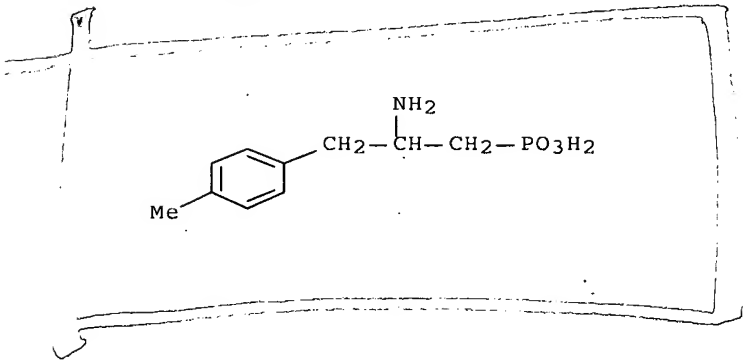
SOURCE: European Journal of Organic Chemistry (1998), (7), 1413-1423
CODEN: EJOCFK; ISSN: 1434-193X
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 129:216686

AB A simple and stereoselective synthesis of primary (E)-allylamines and N-phosphorylated 1-azadienes is reported. N-phosphorylated azadienes were obtained by addn. of ClPPh2 or ClP(OEt)2 to .alpha.,.beta.-unsatd. oximes, while N-(4-methoxyphenyl) azadienes were prepd. by olefination of .beta.-enamino phosphine oxides. Redn. of azadienes and derivs. with hydrides, followed by deprotection of the resulting amines gives primary allylamines and .beta.-amino phosphine oxides, phosphonates, and phosphonic acid derivs.

IT 212388-24-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of N-phosphorylated azadienes, primary allylamines, and .beta.-amino phosphine oxides and -phosphonates from oximes)

RN 212388-24-4 CAPLUS

CN Phosphonic acid, [2-amino-3-(4-methylphenyl)propyl]- (9CI) (CA INDEX NAME)



102(b)

=>

---Logging off of STN---

=>
Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	44.51	581.09

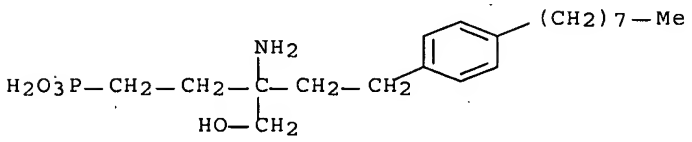
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-6.24	-6.24

sphingosine-1-phosphate (S1P) and by a phosphoryl metabolite of the immunosuppressive agent FTY720. Both species were high-affinity agonists of at least four of the five S1P receptors. These agonists produce lymphopenia in blood and thoracic duct lymph by sequestration of lymphocytes in lymph nodes, but not spleen. S1P receptor agonists induced emptying of lymphoid sinuses by retention of lymphocytes on the abluminal side of sinus-lining endothelium and inhibition of egress into lymph. Inhibition of lymphocyte recirculation by activation of S1P receptors may result in therapeutically useful immunosuppression.

IT 402615-93-4
RL: PAC (Pharmacological activity); BIOL (Biological study)
(alteration of lymphocyte trafficking by sphingosine-1-phosphate receptor agonists)

RN 402615-93-4 CAPLUS

CN Phosphonic acid, [3-amino-3-(hydroxymethyl)-5-(4-octylphenyl)pentyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:171909 CAPLUS Full-text

DOCUMENT NUMBER: 136:216887

TITLE: Preparation of phosphate derivatives as immunosuppressants

INVENTOR(S): Mandala, Suzanne; Bergstrom, James; Hajdu, Richard; Rosen, Hugh; Parsons, William H.; Card, Deborah J.; Maccoss, Malcolm

PATENT ASSIGNEE(S): Merck & Co., Inc., USA

SOURCE: PCT Int. Appl., 59 pp.
CODEN: PIXXD2

103(a) → 102(e)

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

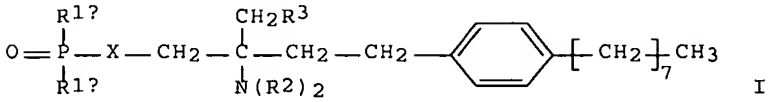
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002018395	A1	20020307	WO 2001-US26789	20010828
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2421893	A1	20020307	CA 2001-2421893	20010828
AU 2001085331	A5	20020313	AU 2001-85331	20010828

EP 1315735	A1	20030604	EP 2001-964485		20010828
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
JP 2004507552	T	20040311	JP 2002-523910		20010828
US 2002091105	A1	20020711	US 2001-942411		20010830
US 6437165	B2	20020820			
PRIORITY APPLN. INFO.:			US 2000-229438P	P	20000831
			WO 2001-US26789	W	20010828

OTHER SOURCE(S): MARPAT 136:216887

GI



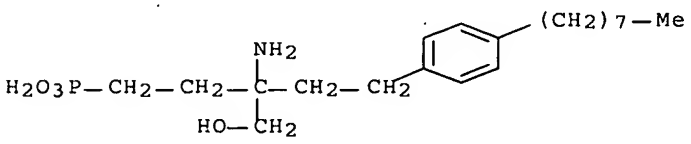
I

AB Immunoregulatory compds. [I; wherein: X = O, S, NR1, (CH2)1-2, optionally substituted with 1-4 halo groups (R1 = H, (C1-C4)alkyl, (C1-C4)haloalkyl); R1a = H, OH, (C1-C4)alkyl,(C1-C4)alkyloxy, the alkyl and alkyloxy portions being optionally substituted with 1-3 halo groups; R1b = H, OH, (C1-C4)alkyl, (C1-C4)haloalkyl; R2 = H, (C1-C4)alkyl, (C1-C4)haloalkyl; and R3 = H, OH, halo, (C1-C4)alkyloxy, (C1-C4)haloalkyloxy], as well as the pharmaceutically acceptable salts and hydrates thereof, are disclosed. Thus, a multistep prepn. of 3-amino-3-hydroxymethyl-5-(4- octylphenyl)pentylphosphonic acid is described. The compds. are useful as immunosuppressants, particularly in the treatment of bone marrow and organ transplant rejection. Pharmaceutical compns. and methods of use are included.

IT 402615-93-4P 402615-95-6P 402615-99-0P
402616-00-6P 402616-04-0P 402616-06-2P
402616-10-8P 402616-11-9P 402616-14-2P
402616-15-3P 402616-18-6P 402616-20-0P
402616-25-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of phosphate derivs. as immunosuppressants)

RN 402615-93-4 CAPLUS

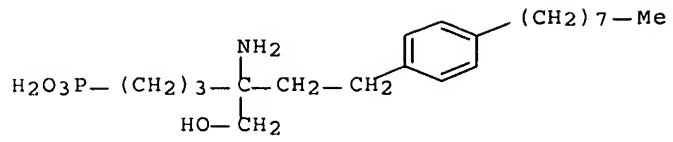
CN Phosphonic acid, [3-amino-3-(hydroxymethyl)-5-(4-octylphenyl)pentyl]- (9CI) (CA INDEX NAME)



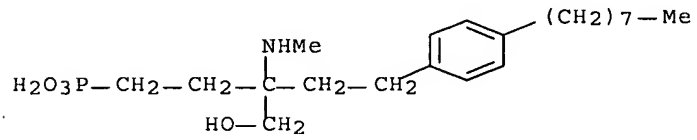
RN 402615-95-6 CAPLUS

CN Phosphonic acid, [4-amino-4-(hydroxymethyl)-6-(4-octylphenyl)hexyl]- (9CI)

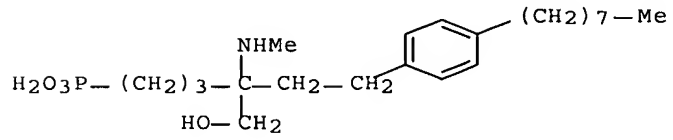
(CA INDEX NAME)



RN 402615-99-0 CAPLUS
CN Phosphonic acid, [3-(hydroxymethyl)-3-(methylamino)-5-(4-octylphenyl)pentyl]- (9CI) (CA INDEX NAME)



RN 402616-00-6 CAPLUS
CN Phosphonic acid, [4-(hydroxymethyl)-4-(methylamino)-6-(4-octylphenyl)hexyl]- (9CI) (CA INDEX NAME)



RN 402616-04-0 CAPLUS
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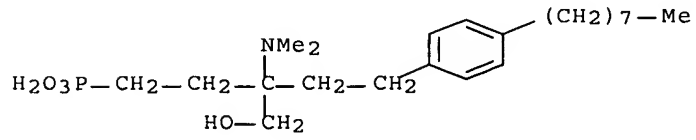
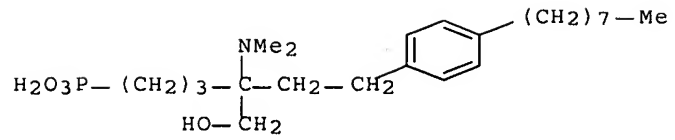
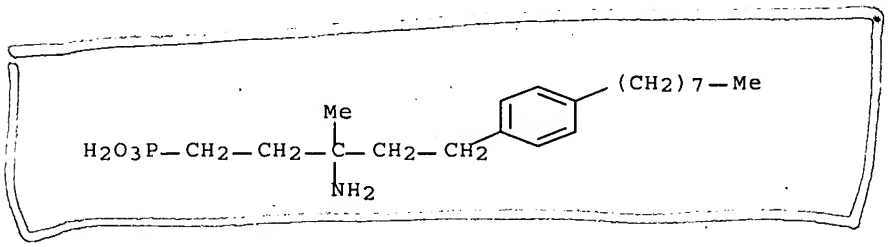


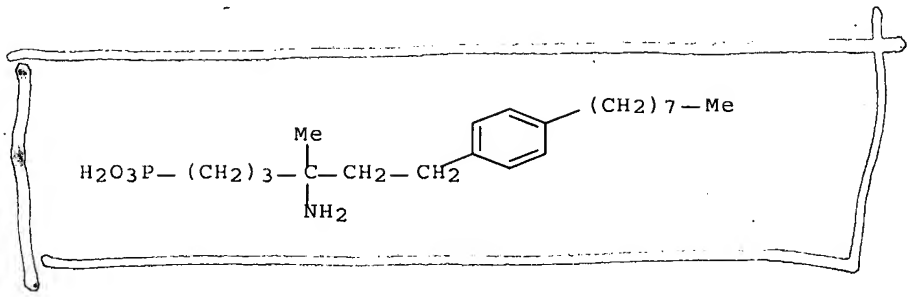
RN 402616-06-2 CAPLUS
CN Phosphonic acid, [4-(dimethylamino)-4-(hydroxymethyl)-6-(4-octylphenyl)hexyl]- (9CI) (CA INDEX NAME)



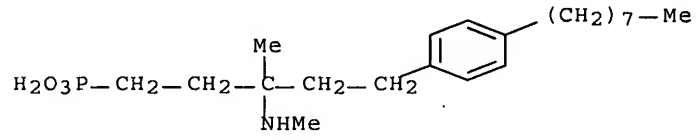
RN 402616-10-8 CAPLUS
CN Phosphonic acid, [3-amino-3-methyl-5-(4-octylphenyl)pentyl]- (9CI) (CA INDEX NAME)



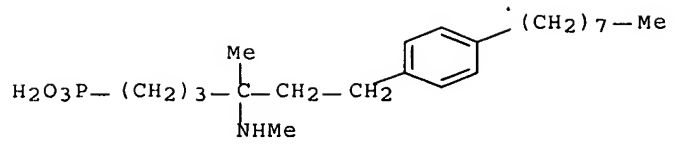
RN 402616-11-9 CAPLUS
CN Phosphonic acid, [4-amino-4-methyl-6-(4-octylphenyl)hexyl]- (9CI) (CA INDEX NAME)



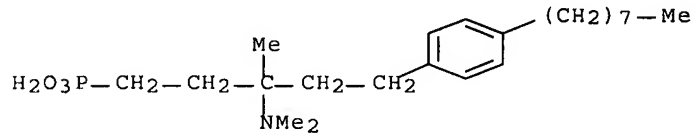
RN 402616-14-2 CAPLUS
CN Phosphonic acid, [3-methyl-3-(methylamino)-5-(4-octylphenyl)pentyl]- (9CI) (CA INDEX NAME)



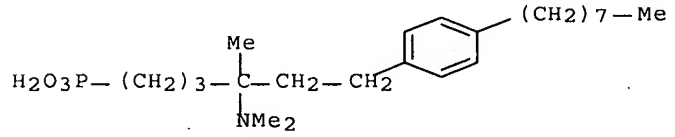
RN 402616-15-3 CAPLUS
CN Phosphonic acid, [4-methyl-4-(methylamino)-6-(4-octylphenyl)hexyl]- (9CI) (CA INDEX NAME)



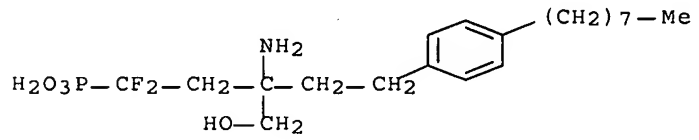
RN 402616-18-6 CAPLUS
CN Phosphonic acid, [3-(dimethylamino)-3-methyl-5-(4-octylphenyl)pentyl]- (9CI) (CA INDEX NAME)



RN 402616-20-0 CAPLUS
CN Phosphonic acid, [4-(dimethylamino)-4-methyl-6-(4-octylphenyl)hexyl]- (9CI) (CA INDEX NAME)



RN 402616-25-5 CAPLUS
CN Phosphonic acid, [3-amino-1,1-difluoro-3-(hydroxymethyl)-5-(4-octylphenyl)pentyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:455564 CAPLUS Full-text
DOCUMENT NUMBER: 129:216686
TITLE: An efficient synthesis of N-phosphorylated azadienes,

primary (E)-allylamines, and .beta.-amino phosphine oxides and -phosphonates from .beta.-functionalized oxime derivatives

AUTHOR(S): Palacios, Francisco; Aparicio, Domitila; Garcia, Jesus; Rodriguez, Encina

CORPORATE SOURCE: Departamento Quimica Organica, Facultad Farmacia, Universidad Pais Vasco, Vitoria, E-01080, Spain

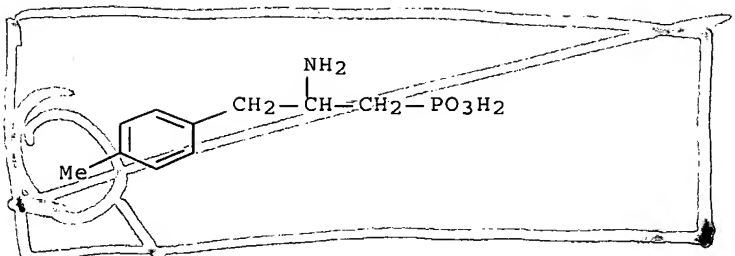
SOURCE: European Journal of Organic Chemistry (1998), (7), 1413-1423
CODEN: EJOCFK; ISSN: 1434-193X
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 129:216686

AB A simple and stereoselective synthesis of primary (E)-allylamines and N-phosphorylated 1-azadienes is reported. N-phosphorylated azadienes were obtained by addn. of ClPPh2 or ClP(OEt)2 to .alpha.,.beta.-unsatd. oximes, while N-(4-methoxyphenyl) azadienes were prepd. by olefination of .beta.-enamino phosphine oxides. Redn. of azadienes and derivs. with hydrides, followed by deprotection of the resulting amines gives primary allylamines and .beta.-amino phosphine oxides, phosphonates, and phosphonic acid derivs.

IT 212388-24-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of N-phosphorylated azadienes, primary allylamines, and .beta.-amino phosphine oxides and -phosphonates from oximes)

RN 212388-24-4 CAPLUS

CN Phosphonic acid, [2-amino-3-(4-methylphenyl)propyl]- (9CI) (CA INDEX NAME)



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---Logging off of STN---

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Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	44.51	581.09

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-6.24	-6.24